From High Throughput to High Difficulty: The Evolution of Protein Crystallography for Drug Discovery

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Structure-based drug design (SBDD) has been used with increasing success during the past decade for the discovery of potent and selective molecules to target various diseases. Protein crystallography carried out at synchrotron beamlines is the main SBDD tool used today. The various automation tools developed at the height of the structural genomics efforts helped also to establish high-throughput crystallography for drug discovery efforts, enabling the structure determination of large numbers of protein-ligand co-complex structures. During this talk some of the recent technical breakthroughs in x-ray and beamline technologies will be reviewed, such as microfocus beams and advanced software tools, which are benefitting the pharmaceutical industry to tackle drug targets with increasing difficulties. An SBDD case study will be also presented.